

# **Multi-Step Combustion Model for FDS**

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**FIRE SCIENCE & ENGINEERING**

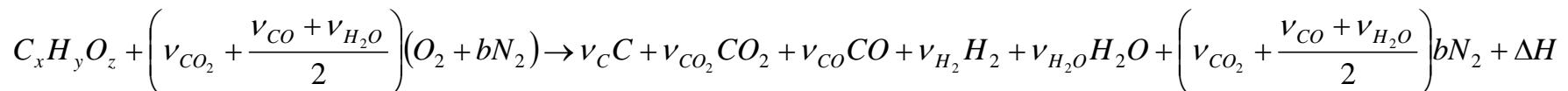
# Topics

- Background
- Two-parameter mixture fraction
- Validation testing
  - ◆ Methane slot burner (Norton, Smyth, Miller, & Smooke)
  - ◆ Beyler's hood experiments
  - ◆ Reduced Scale Enclosure experiments
    - Original series (Bryner, Johnsson, & Pitts)
    - New series (Johnsson, Bundy, Hamins, & Lenhert)



# Background

- FDS v2 – v4 use a single parameter mixture fraction where the user specifies a single chemical reaction:



- Good for scenarios with well ventilated fires
- For steady state under ventilated fires this approach typically results in excessive temperatures unless the user provides a reaction input representation of the degree of under ventilation. However:
  - ◆ The early well ventilated portion of the fire is no longer represented well.
  - ◆ Uncertainties in how to appropriately specify the reaction for scenarios with complex ventilation (e.g. more complex than a hood or a box with a single door).



# Background (2)

- Interested in a method to predict CO formation
  - ◆ Minimize use of user defined “tuning knobs”
  - ◆ Minimize computational expense
  - ◆ Maximize potential to add future capabilities with minimum restructuring



# Approach

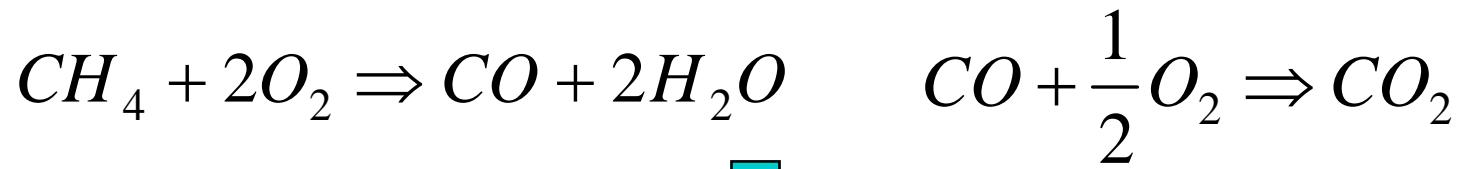
- Examine potential to use 2-reaction chemistry:



- Stay within a mixture fraction framework to reduce the number of transport equations



# Two-parameter Mixture Fraction



$$\frac{DY_{CH_4}}{Dt} = \nabla \cdot \rho D \nabla Y_{CH_4} + \dot{m}_{CH_4,1}'''$$

$$\frac{DY_{CO}}{Dt} = \nabla \cdot \rho D \nabla Y_{CO} + \dot{m}_{CO,1}''' + \dot{m}_{CO,2}'''$$

$$\frac{DY_{CO_2}}{Dt} = \nabla \cdot \rho D \nabla Y_{CO_2} + \dot{m}_{CO_2,2}'''$$



$$Z_1, Z_2$$

# Two-parameter Mixture Fraction

$$Z_1 + Z_2 = Y_{CH_4} + \frac{W_{CH_4}}{W_{CO}} Y_{CO} + \frac{W_{CH_4}}{W_{CO_2}} Y_{CO_2}$$

Mass of unburned fuel      Mass of fuel converted to CO      Mass of fuel converted to  $CO_2$

$$Z_1 + Z_2 = Z$$



# Two-parameter Mixture Fraction

$$\frac{DZ_1}{Dt} = \nabla \cdot \rho D \nabla Z_1 + \frac{W_{CH_4}}{W_{CO}} \dot{m}_{CO,2}'''$$

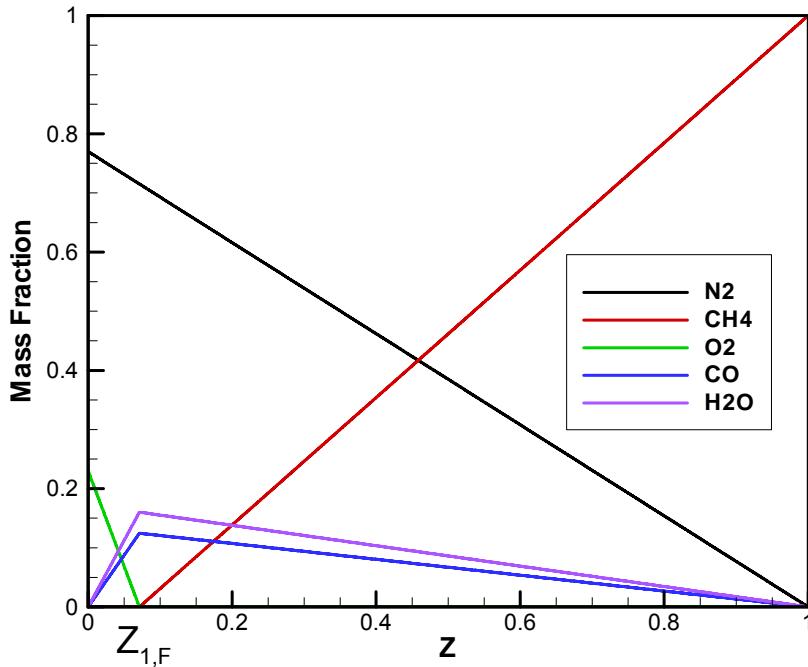
$$\frac{DZ_2}{Dt} = \nabla \cdot \rho D \nabla Z_2 - \frac{W_{CH_4}}{W_{CO}} \dot{m}_{CO,2}'''$$

- Source terms for  $Z_1$  and  $Z_2$  cancel, guarantees mass conservation
- No inherent assumption on the kinetics of the source term, however:
  - ◆ Typical grid resolution won't have flame temperatures

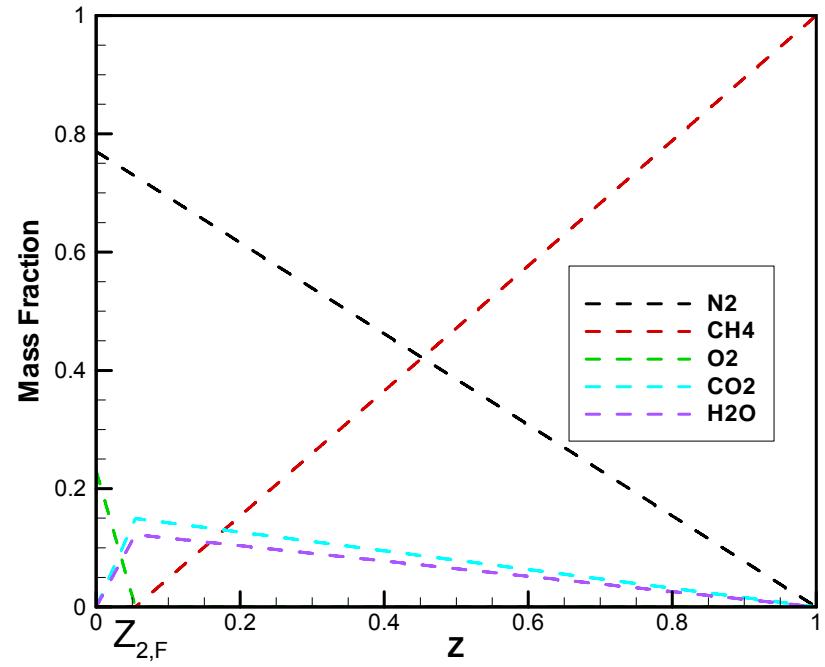


# State Relations

$\text{CH}_4$  to CO



$\text{CH}_4$  to  $\text{CO}_2$



Desire computationally efficient manner to combine the two sets of state relations as function of  $Z_1$  and  $Z_2$ . Note:  $Z_{2,F} < Z_{1,F}$



# State Relations

Define  $c$  as the ratio of  $Z_2$  from the simulation to  $Z_2$  computed using the maximum possible  $Z_2$  for  $Z_1+Z_2$  from the simulation.  $0 \leq c \leq 1$ .

$$c = \frac{Z_2}{Z_{2,max}} = \frac{Z_2}{Z_2[Y_{CO_2}(Z_1 + Z_2)]}$$

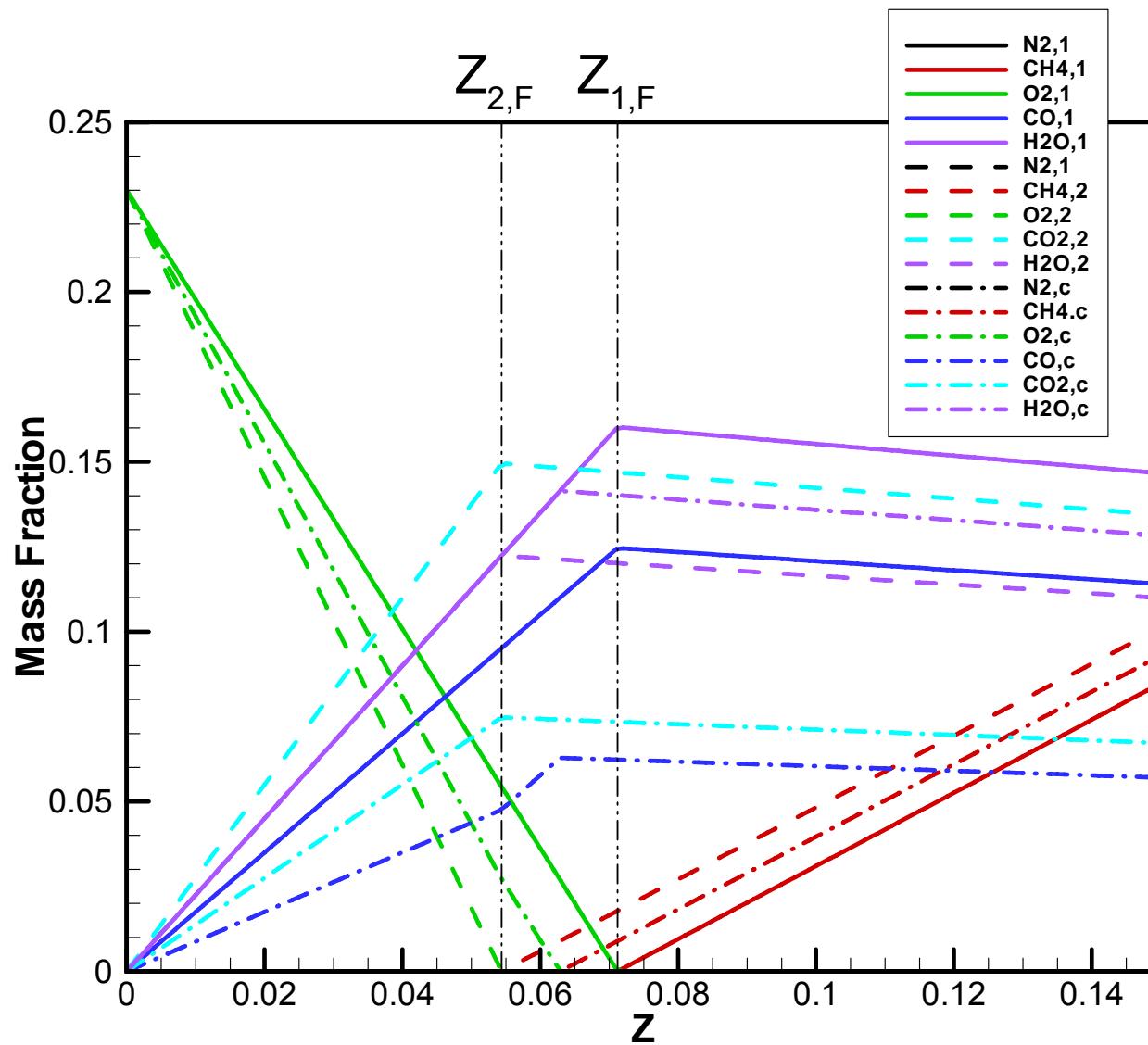
We can then generate state relations as:

$$Y_i(Z_1, Z_2) = (1 - c)Y_{i,1} + cY_{i,2} + \xi_i(Z_1 + Z_2, c)$$

$\xi_i(Z_1 + Z_2, c)$  accounts for non-linearities between  $Z_{1,F}$  and  $Z_{2,F}$

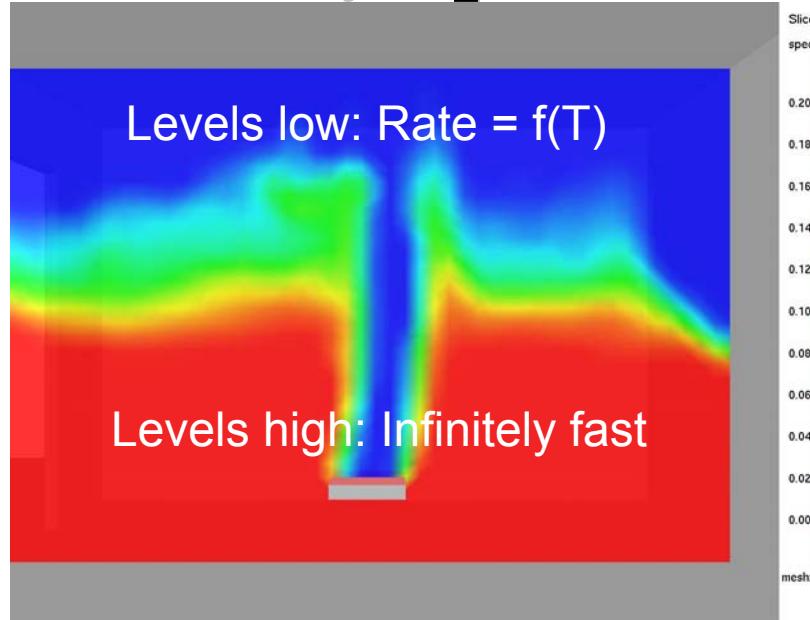


# State Relations c=0.5



# Reaction Kinetics

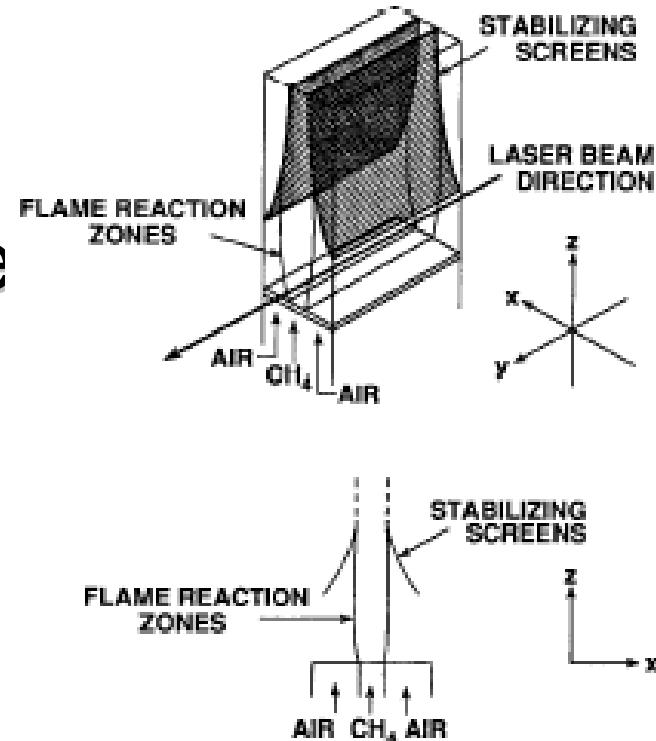
- Reaction 1: Fuel + O<sub>2</sub> → CO + H<sub>2</sub>O
  - ◆ Infinitely fast
- Reaction 2: CO + O<sub>2</sub> → CO<sub>2</sub>
  - ◆ Infinitely fast
  - ◆ Base on nearby O<sub>2</sub> levels



# Wolfhard-Parker Slot Burner (Smyth et al.)

(U)

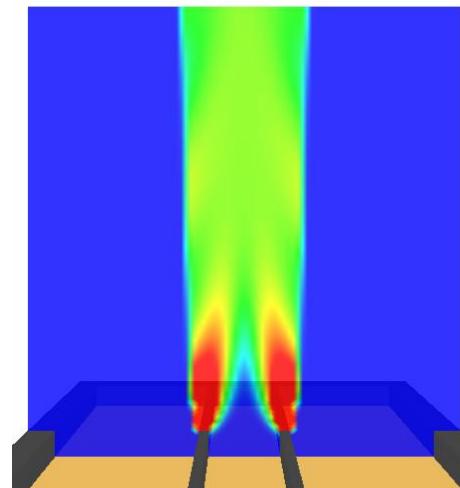
- 2D laminar, methane-air, diffusion flame
- Measured temperature and many major and minor species at elevations near the burner surface



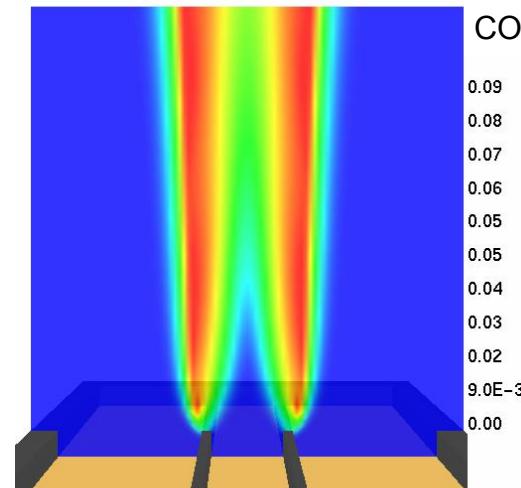
# Slot Burner – FDS v5α

Smokeview 4.0.6 – Sep 15 2005

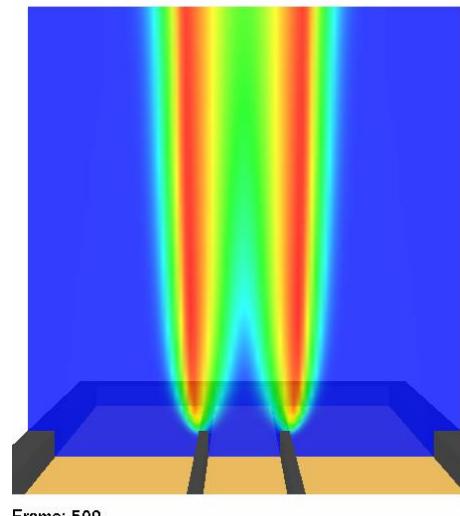
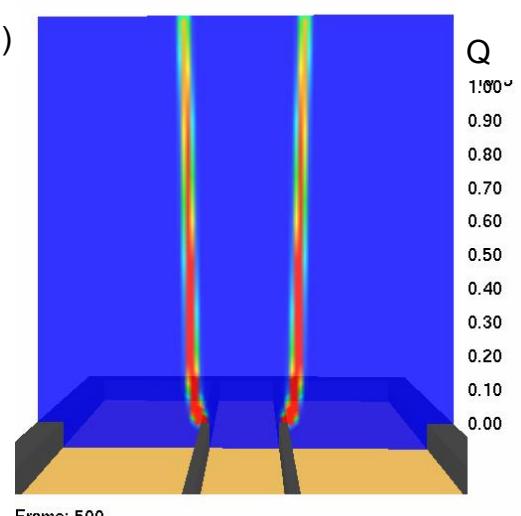
Smokeview 4.0.6 – Sep 15 2005

Frame: 501  
Time: 1.002

Smokeview 4.0.6 – Sep 15 2005

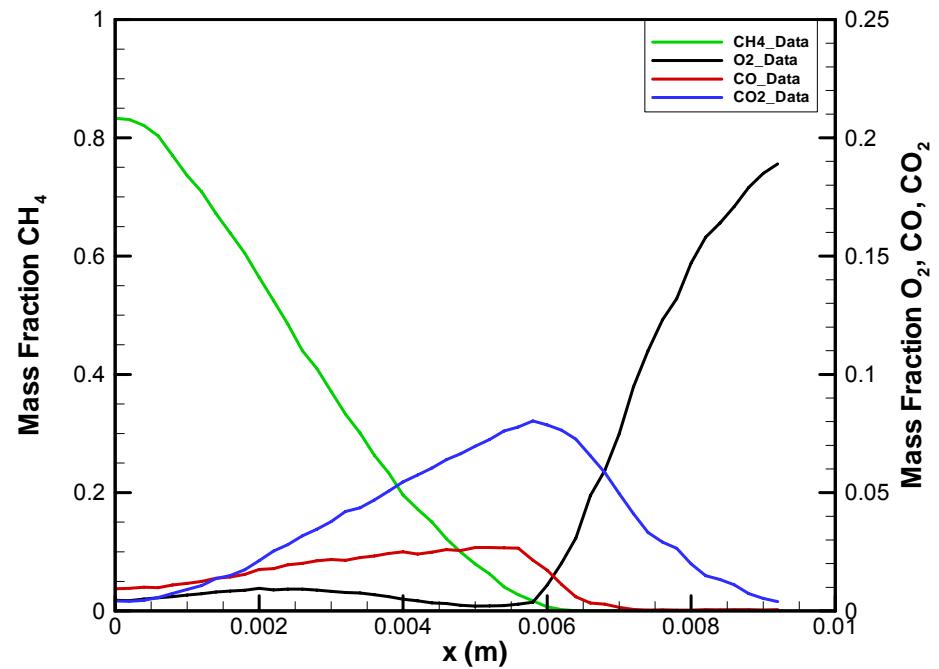
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Time: 1.000

Smokeview 4.0.6 – Sep 15 2005

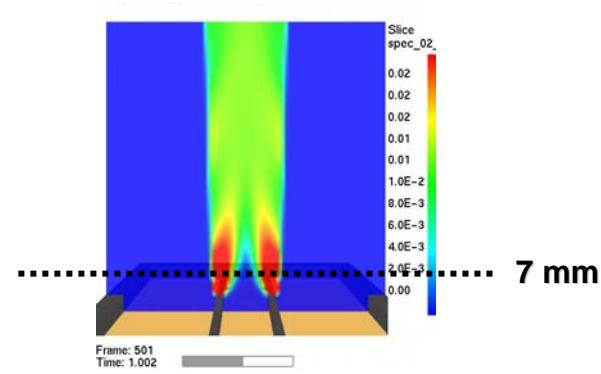
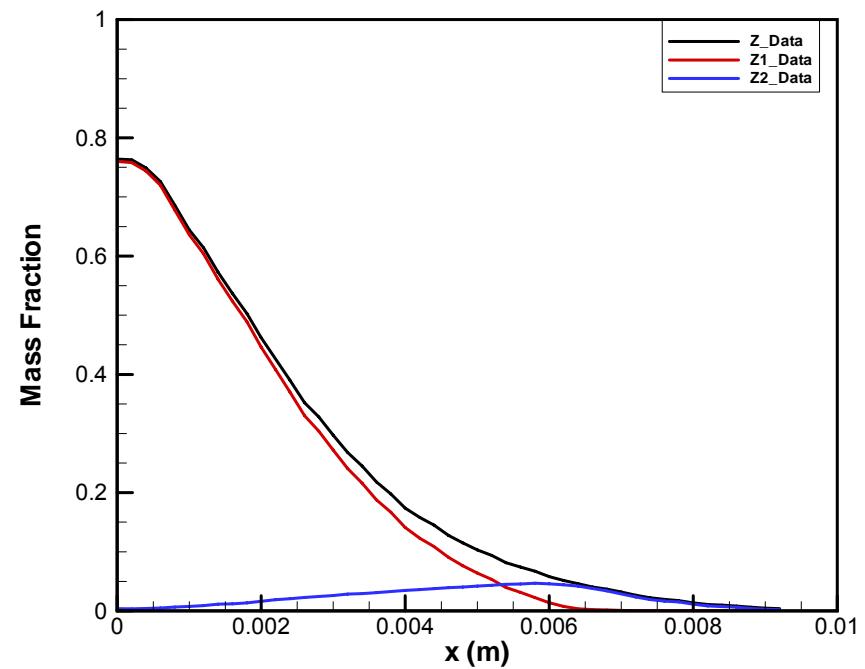
Frame: 509  
Time: 1.018Frame: 500  
Time: 1.000

# Data

7 mm Above Burner

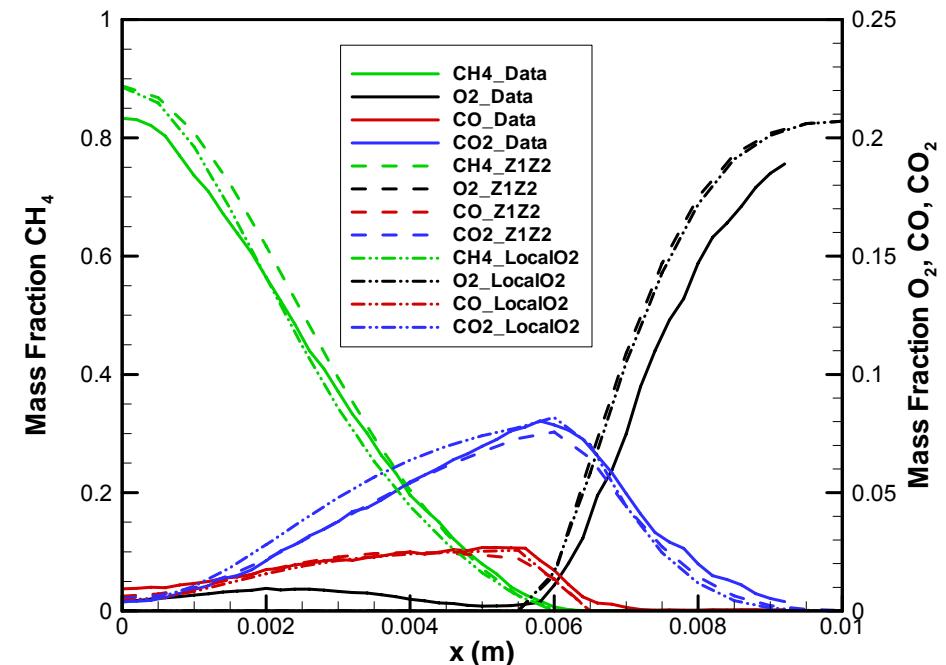


7 mm Above Burner

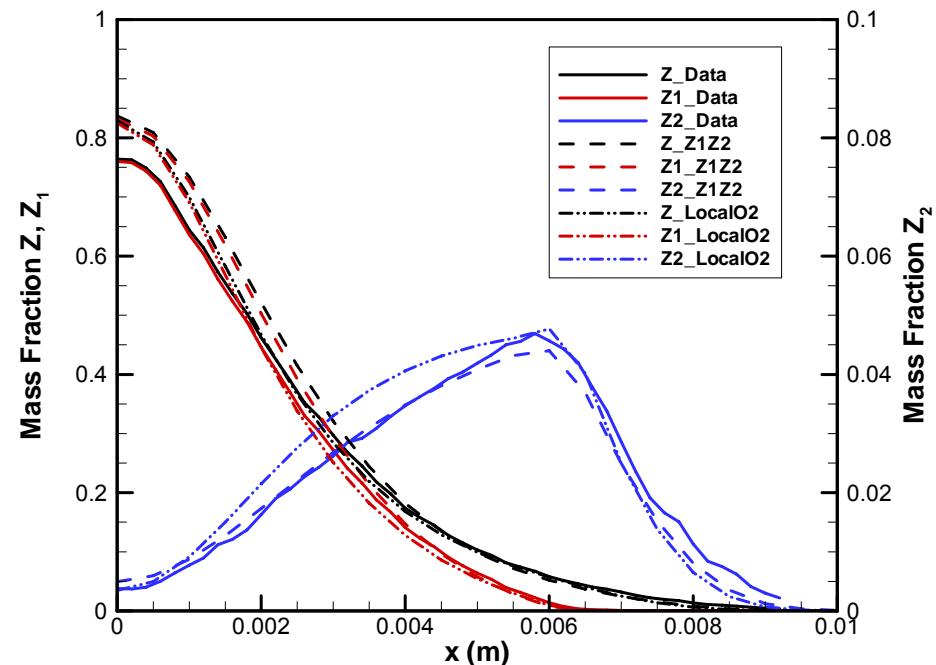


# Results

7 mm Above Burner

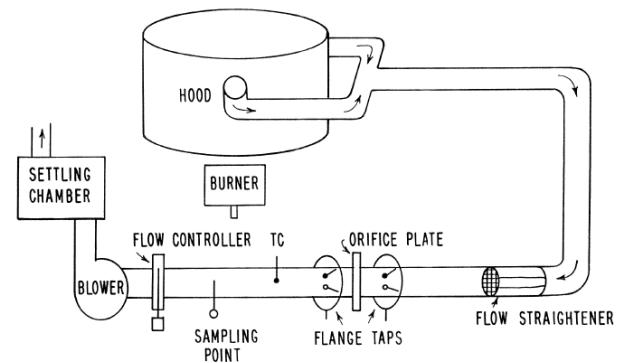
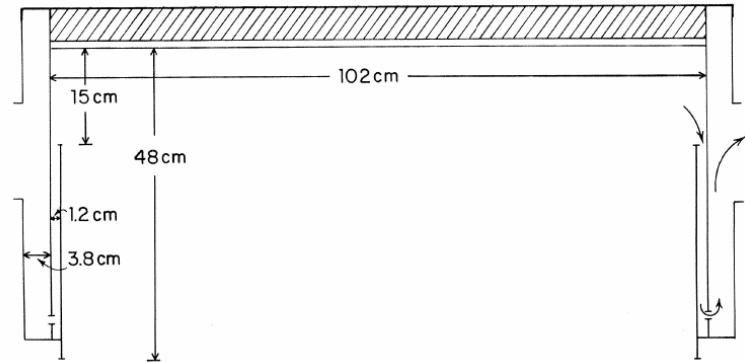


7 mm Above Burner



# Beyler Hood

- Adjustable height burner located beneath a hood
- Varied distance from hood lip to burner surface, burner diameter, fuel, and fire size
- Hood exhaust rate manually controlled to prevent spill from the hood lip
- Measured gas concentrations in the exhaust duct

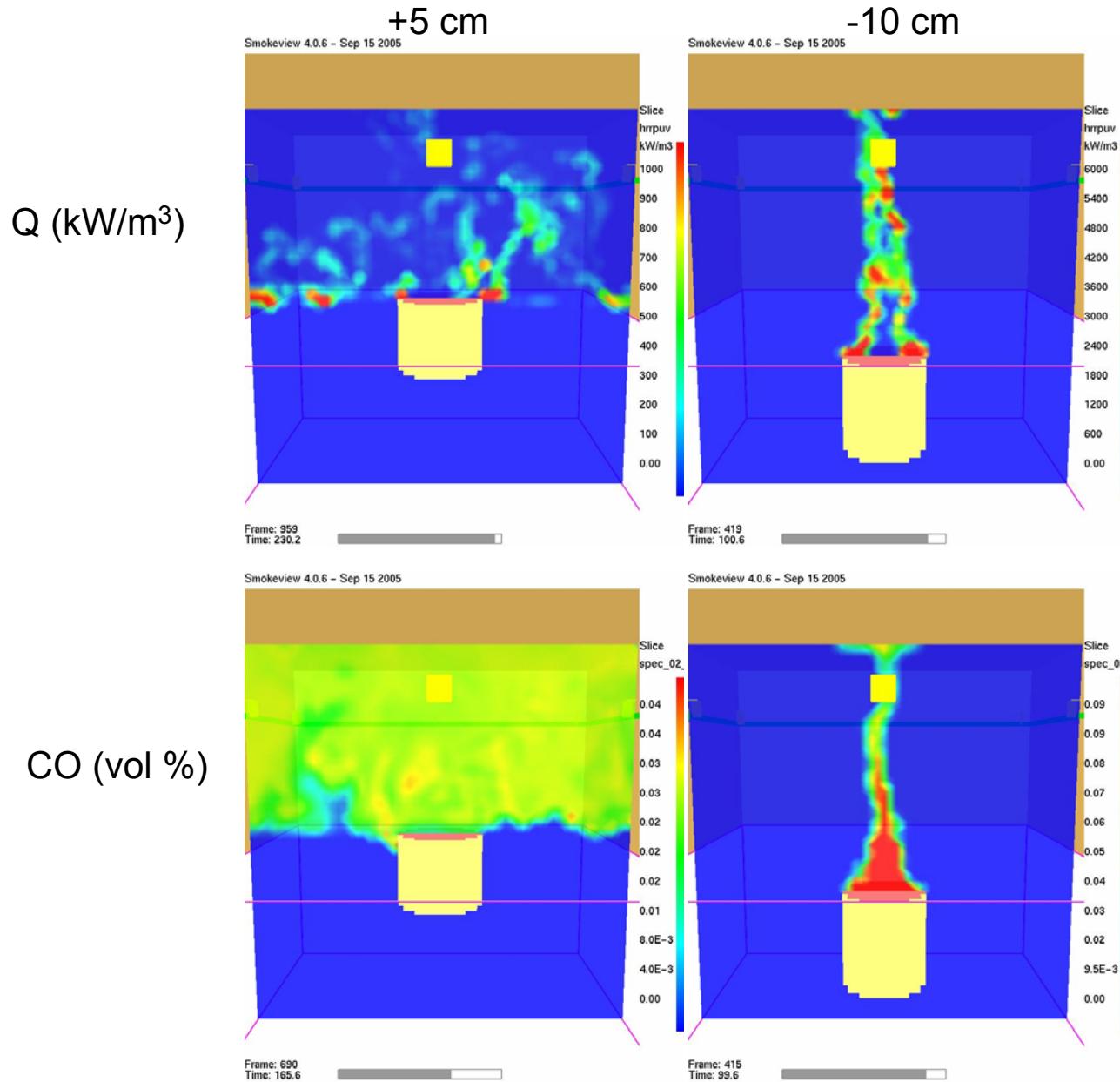


# Simulations Performed

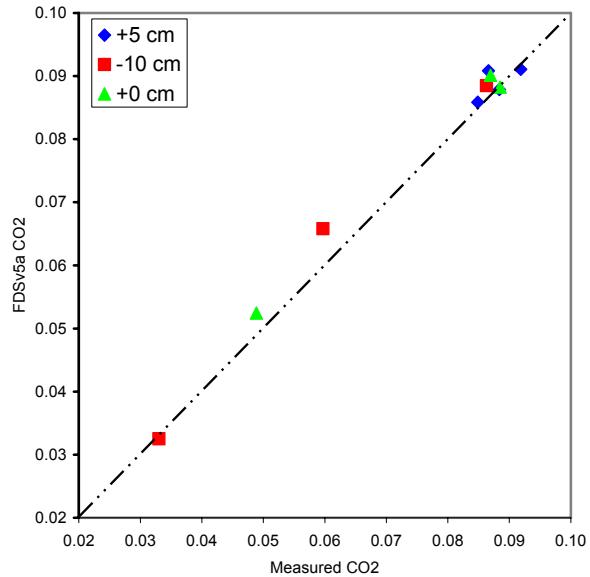
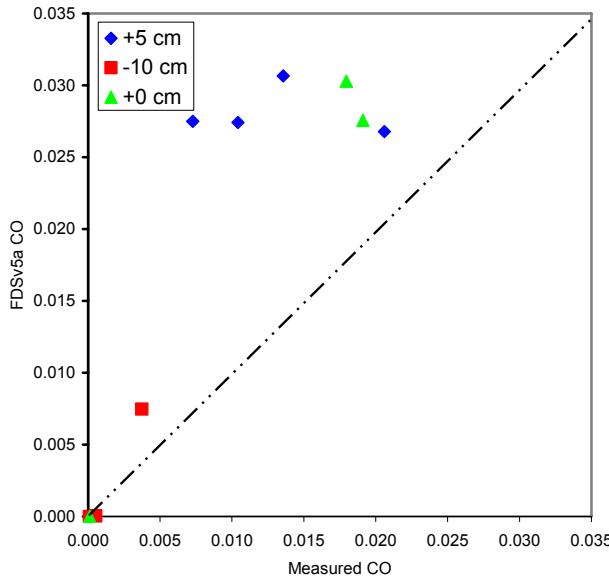
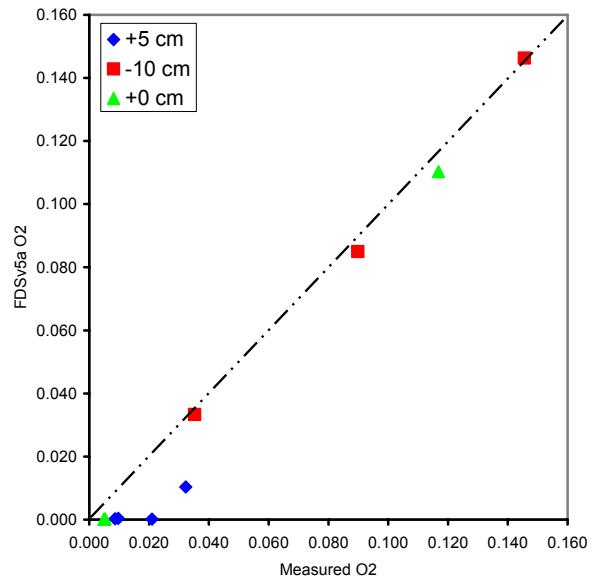
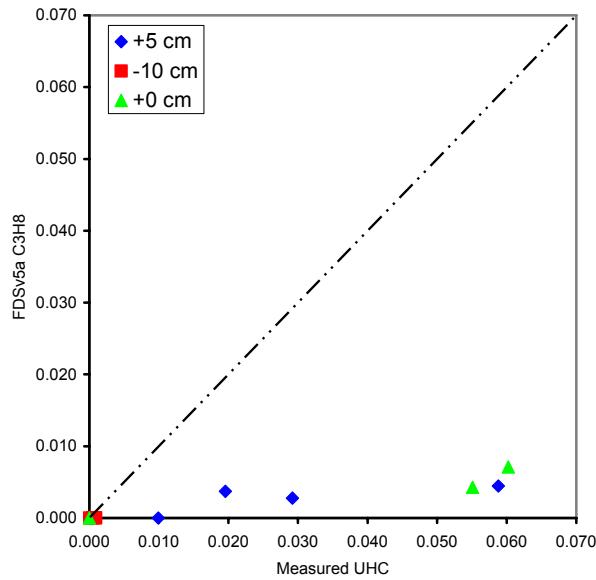
- 19 cm burner, propane
  - ◆ 5 cm above hood lip
    - 7.92 kW, 13.53 kW, 18.25 kW, 24.30 kW
  - ◆ 0 cm above hood lip
    - 8.21 kW, 18.25 kW, 31.52 kW
  - ◆ 10 cm below hood lip
    - 8.21 kW, 18.25 kW, 24.30 kW
- Two step, finite rate with CO based on local O<sub>2</sub>



# Results – 18.25 kW

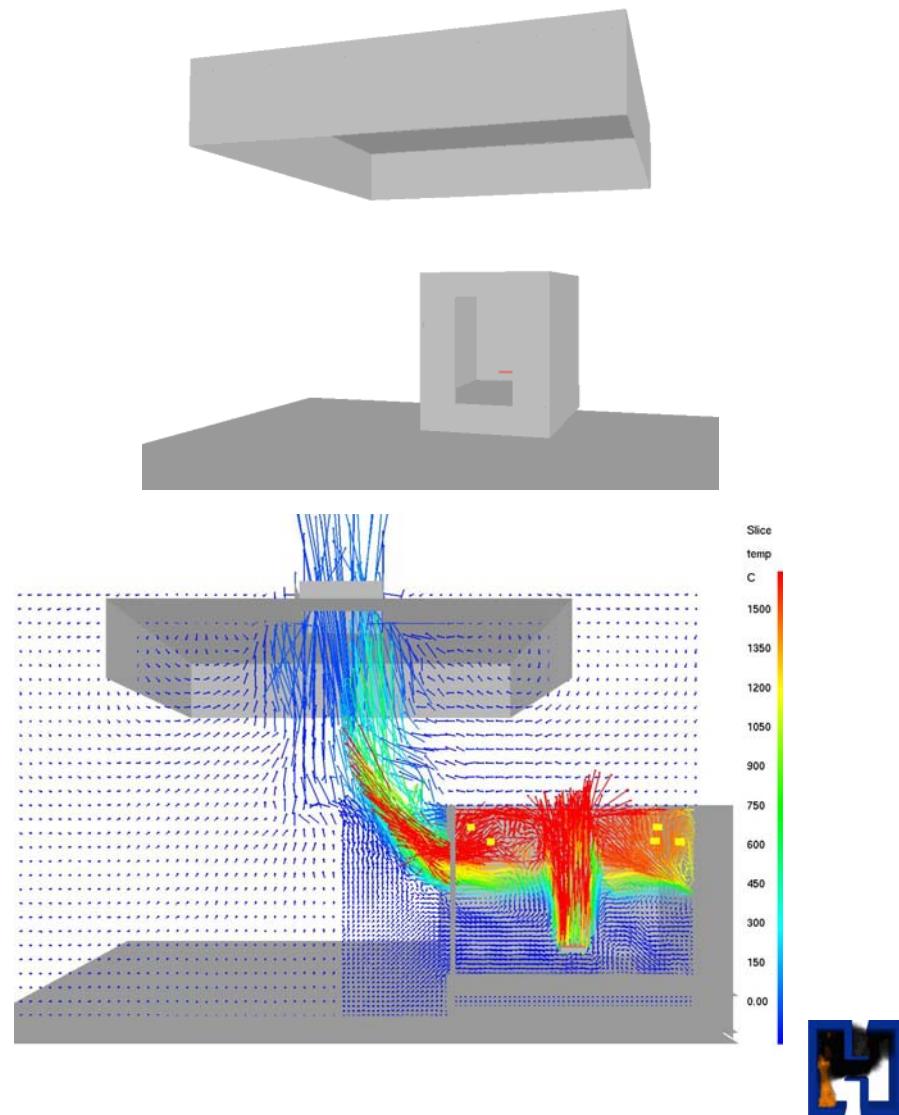


# Results



# RSE Experiments (Bryner, et al.)

- 40 % of an ISO-9705 room
- Elevated methane burner
- Gas concentration measurements in upper layer at front and back of compartment



# Simulations Performed

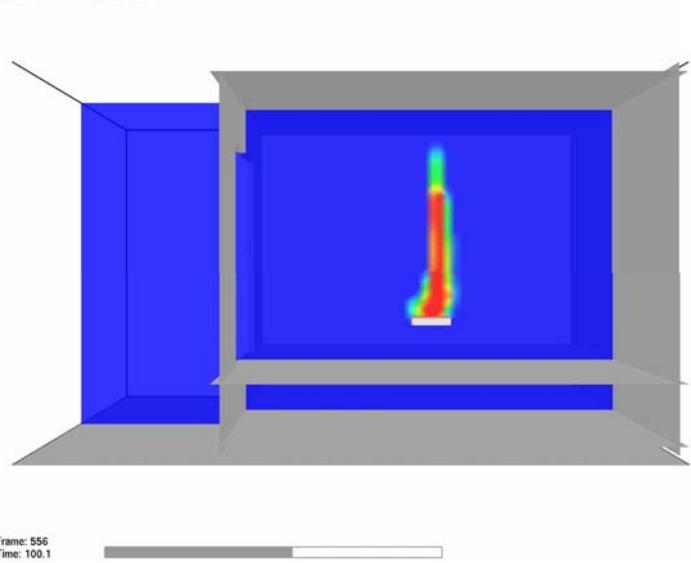
- FDSv4 – CO *prescribed*
  - ◆ well ventilated species yields
  - ◆ under ventilated species yields
- FDSv5 $\alpha$  – CO *computed*
  - ◆ two parameter
  - ◆ finite rate
    - CO = always fast
    - CO =  $f(O_2, T)$



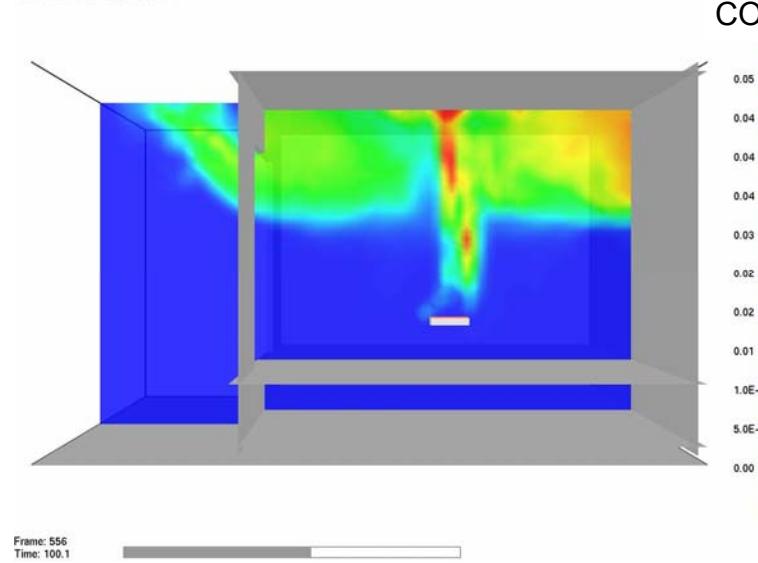
(U)

# 50 kW – Finite Rate $f(O_2, T)$

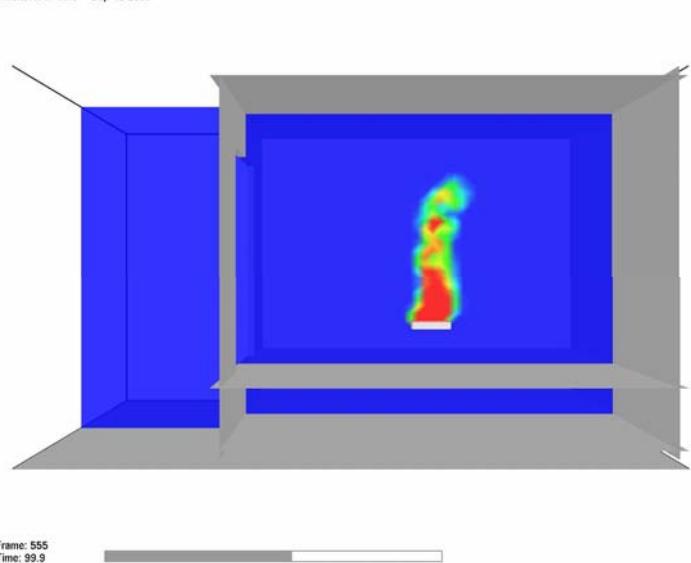
Smokeview 4.0.6 – Sep 15 2005



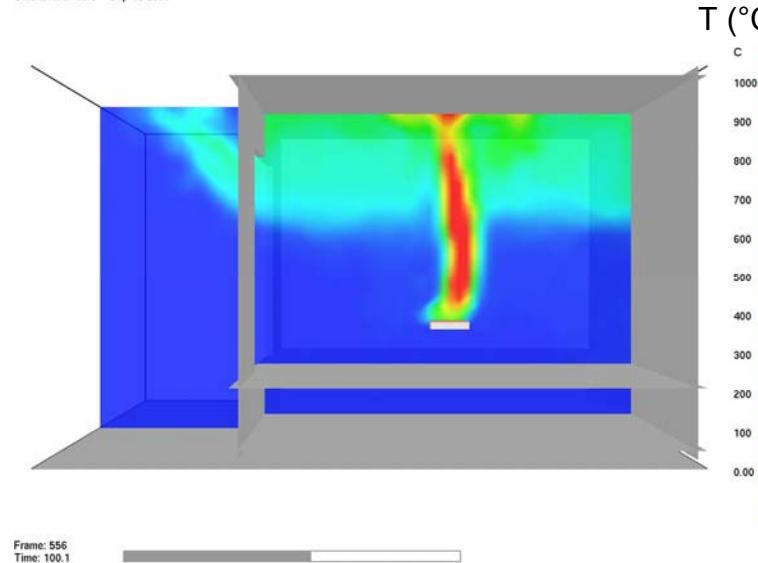
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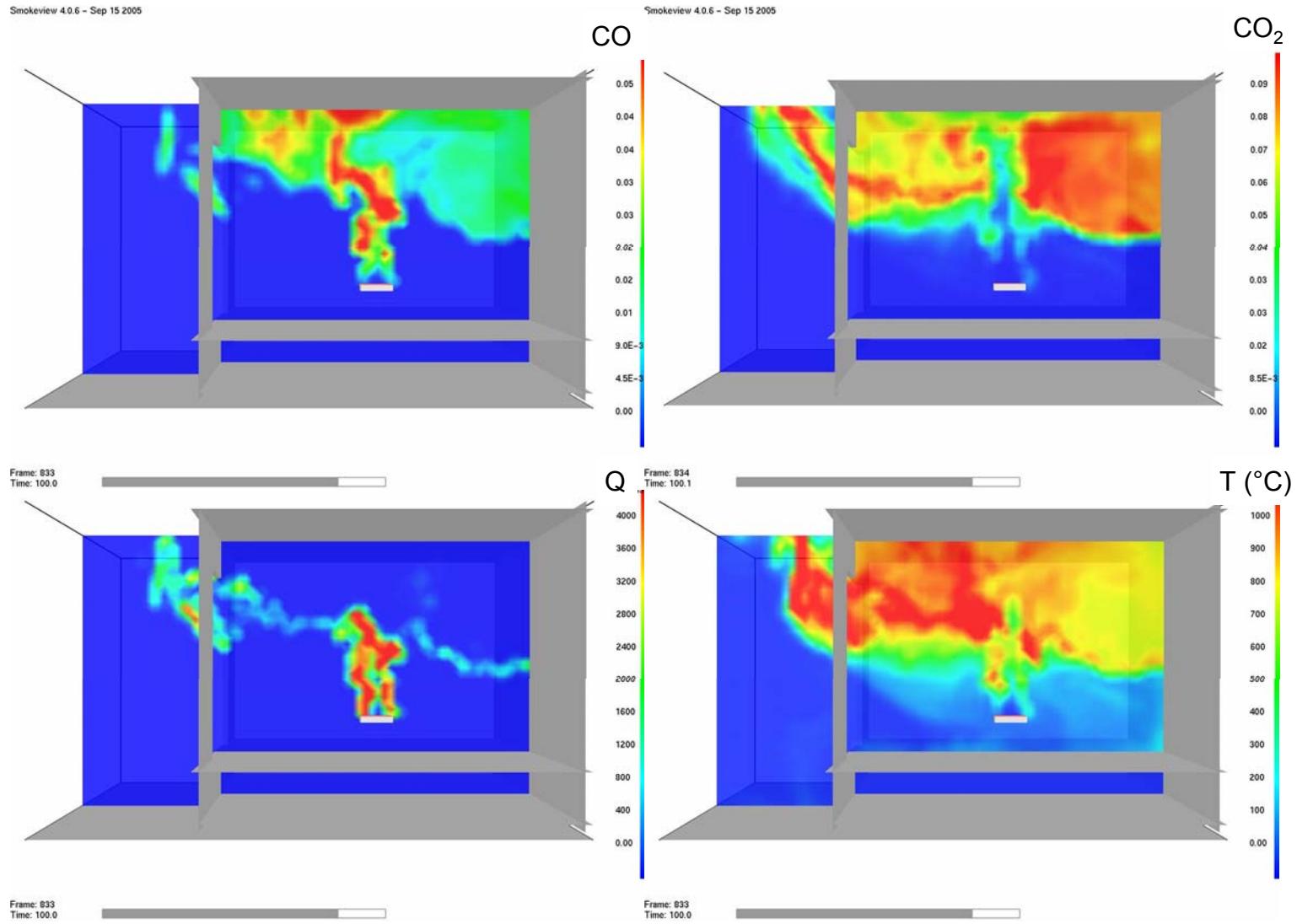
Smokeview 4.0.6 – Sep 15 2005



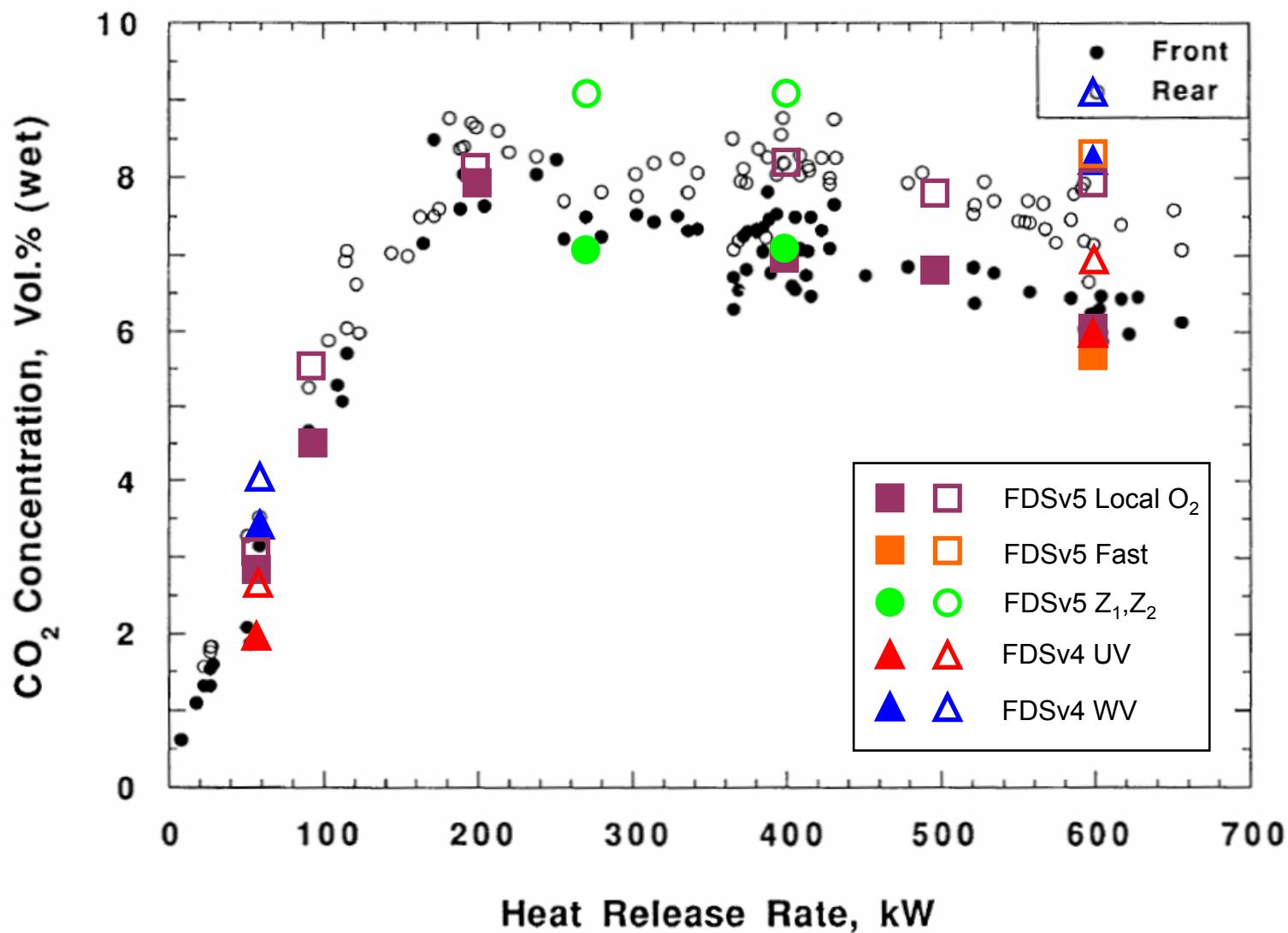
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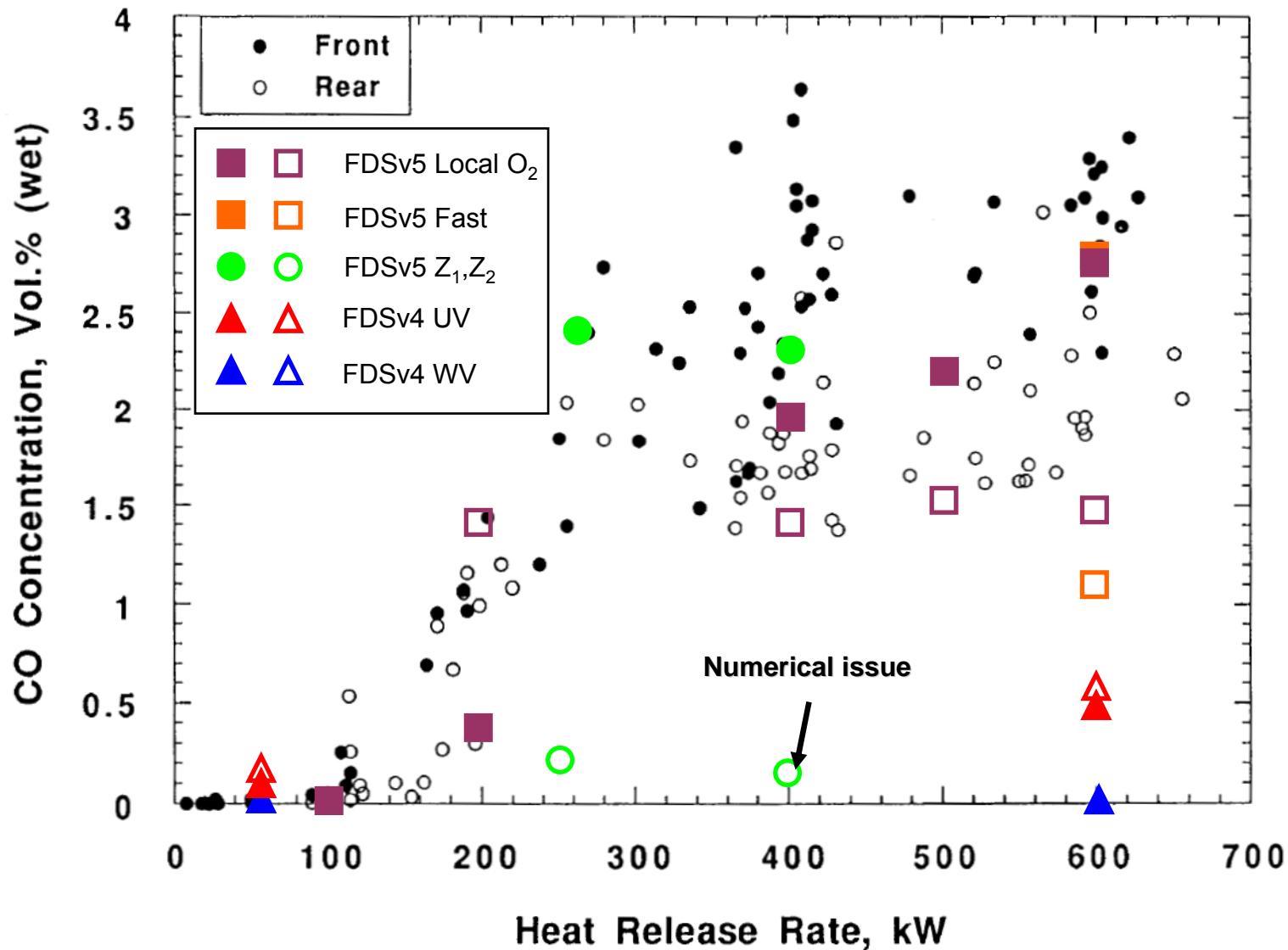
# 400 kW – Finite Rate $f(O_2, T)$



# $\text{CO}_2$ : FDS v4 + v5 vs. Data (Bryner et al.)

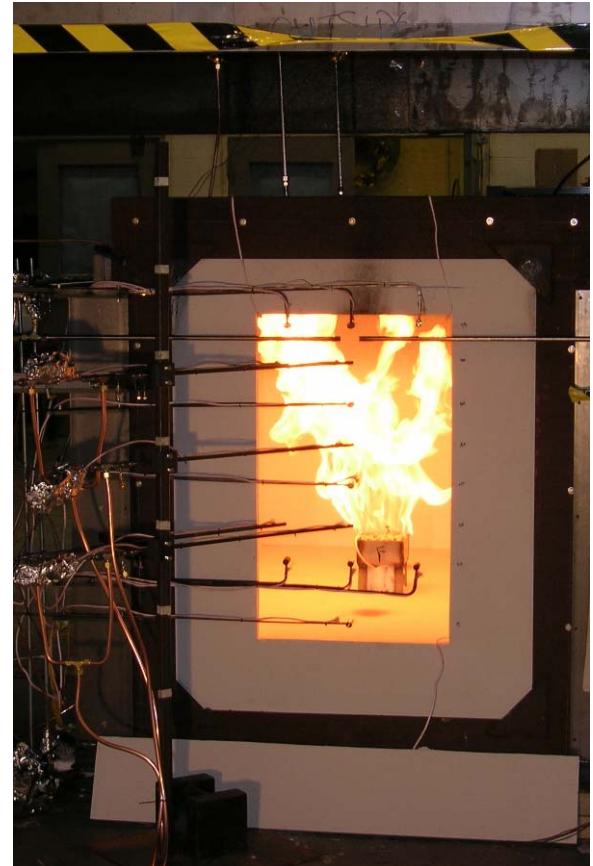


# CO: FDS v4 + v5 vs. Data (Bryner et al.)

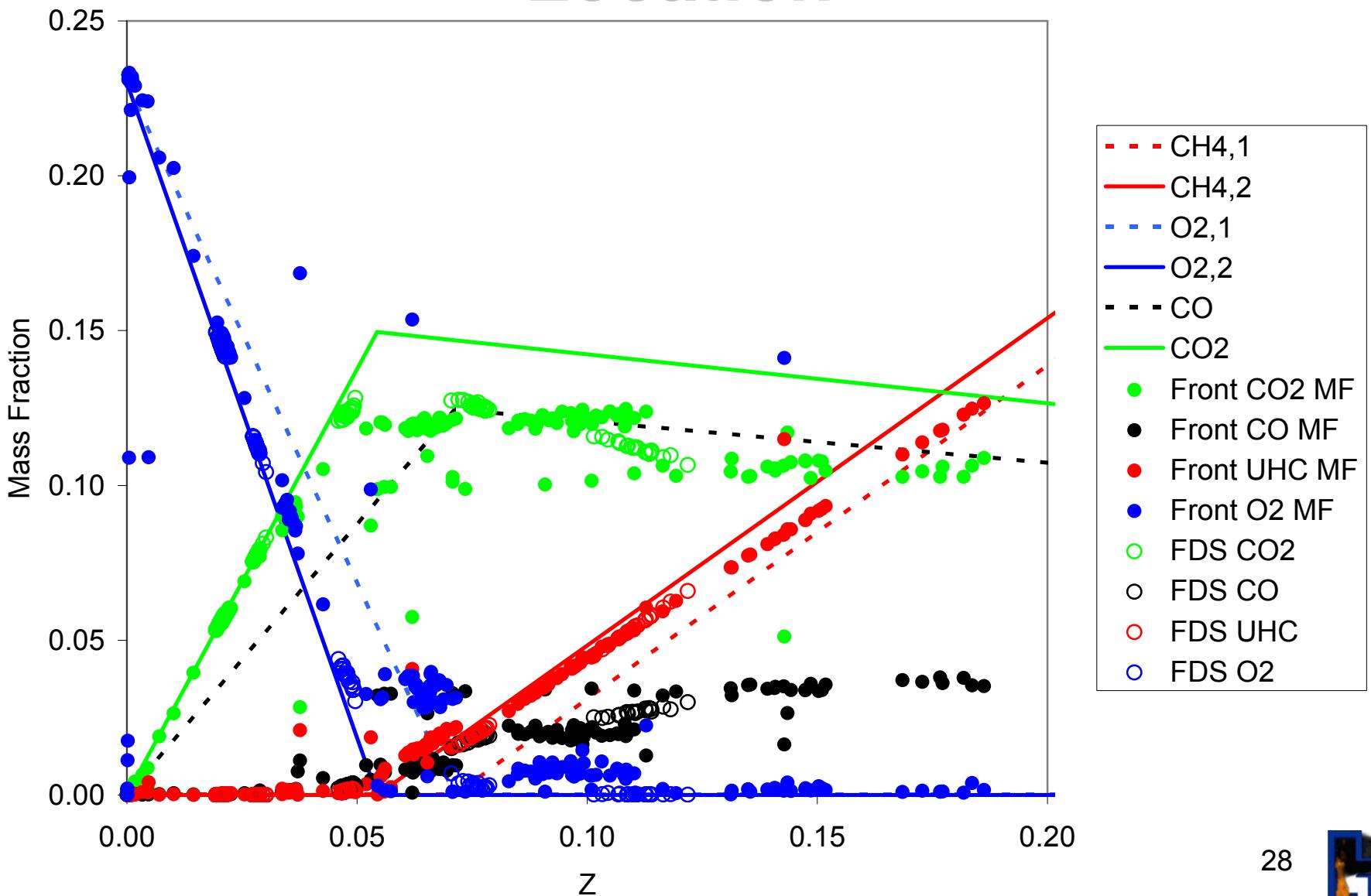


# New RSE Tests (Johnsson, et al.)

- Currently conducting testing using RSE
- Primary goal to reduce dataset uncertainties for use as FDS validation
- *Preliminary* dataset
  - ◆ Shakedown test
  - ◆ Operated burner at fixed fire size for ~15 minutes and then changed fire size. Single test includes 75, 115, 180, 270, and 400 kW fires
- Plotted quasi-steady blind FDS predictions along with *transient* test data in Z-space



# New RSE Tests – Front Sample Location



# Still to Do

- Radiation solver details for two-parameter mixture fraction
- Approach for determining  $\dot{m}_{CO,2}'''$  term
- Numerical behavior of two-parameter approach (overshoots/undershoots in mass fractions)
- V&V
- Computational efficiency
- User friendliness

